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Research Article

Distance-Based Topological Polynomials Associated with Zero-Divisor Graphs

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Let R be a commutative ring with nonzero identity and let $Z(R)$ be its set of zero divisors. The zero-divisor graph of R is the graph $\Gamma(R)$ with vertex set $V(\Gamma(R)) = Z(R)^*$, where $Z(R)^* = Z(R)\backslash\{0\}$, and edge set $E(\Gamma(R)) = \{\{x, y\}\colon\ x \cdot y = 0\}$. One of the basic results for these graphs is that $\Gamma(R)$ is connected with diameter less than or equal to 3. In this paper, we obtain a few distance-based topological polynomials and indices of zero-divisor graph when the commutative ring is $\mathbb{Z}_{p^2q^2}$, namely, the Wiener index, the Hosoya polynomial, and the Shultz and the modified Shultz indices and polynomials.

1. Introduction

Algebraic structures have been investigated significantly for their nearby connection with representation theory and number theory; likewise, they have been widely concentrated in combinatorics [1, 2]. Despite the expansive theoretical research in these areas, restricted rings and fields got consideration for their applications to cryptography and coding theory.

In mathematical chemistry, a graphical structure of a chemical compound is a representation of the structural formula. In a chemical graph, vertices and edges represent the atoms and their chemical bonds of the compound, respectively. Molecular descriptors for a particular chemical compound are calculated on basis of the corresponding molecular graph. A topological index is a graph invariant that is obtained from it. In [3], the first topological index, namely, the Wiener index, was introduced. Nowadays, it is widely used in QSAR ("Quantitative Structure Activity Relationship"), whose properties are surveyed in [4, 5].

Topological indices are classified as degree based [6–9] and distance based of graphs. Some well-known topological indices based on the degrees of a graph are the Randić connectivity index, Zagreb indices, Harmonic index, atom bond connectivity, and geometric arithmetic index. The Wiener index, Hosaya index, and Estrada index are distance-based topological indices [10, 11]. Topological indices formulate the criteria for the development of compound structures, and numerical activities on these structures extend multidisciplinary research. In what follows, we cite some of them.

A relationship among the stability of linear alkanes and the branched alkanes is examined using the *ABC* index, which helped in computation of strain energy for cycle alkanes [12, 13]. The GA index is more appropriate and efficient to correlate certain physico-chemical characteristics for predictive power than the Randić connectivity index [14, 15]. The Zagreb indices are powerful tools for the calculation of total p-electron energy of the molecules with precise approximation [16]. The degree-based topological indices are more useful to examine the chemical characteristics of distinct molecular structures. Eccentricity-based topological indices are useful as a key for the judgement of toxicological, physico-chemical, and pharmacological properties of a compound through the structure of its molecules. The study of the QSAR is known for this sort of analysis [17]. By exploring [18, 19], further applications of topological indices can be obtained.

1.1. Distance-Based Topological Indices and Polynomials. In this section, we introduce the topological indices and polynomials that will be obtained for the graphs studied in this paper. We recall some concepts from graph theory. Let G be a (undirected) graph. If there is a path between any two distinct vertices of G, then G is a connected graph. For two distinct vertices $x, y \in V(G)$, we denote $d(x, y)$ the length of a shortest path connecting x and y ($d(x, x) = 0$ and, $d(x, y) = \infty$ if no such a path exists). The diameter of the graph G is the maximum length of the shortest path connecting two distinct vertices of G, that is, $\operatorname{diam}(G) = \max\{d(x, y)\colon\ x \neq y \in V(G)\}$. The number of edges incidence a vertex x of simple graph G is called the degree of the vertex x, denoted as d_x.

The Wiener index [11] was introduced by Wiener in 1947 to illustrate the connection between physico-chemical properties of organic compounds and the index of their molecular graphs:

$$W(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} d(u, v). \tag{1}$$

Randić [20] and Randić et al. [21] introduced a modified version of the Wiener index that is used for predicting physico-chemical properties of organic components. The new index was called the hyper-Wiener index and it is defined as follows:

$$WW(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} \left(d(u, v) + d(u, v)^2\right). \tag{2}$$

The Hosoya polynomial was introduced in 1989 [22]. The definition is as follows:

$$H(G, x) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} x^{d(u,v)}. \tag{3}$$

Dobrynin and Kochetova [23], and independently, Gutman [24] introduced a degree distance index, which is known as the Schultz index. Let G be a connected graph and d_u be the degree of $u \in V(G)$. Then, the Schultz index or the degree distance of G is defined as follows:

$$\operatorname{Sc}(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u + d_v) d(u, v). \tag{4}$$

Klavžar and Gutman defined, in [25], the modified Schulz index of a graph as follows:

$$\operatorname{Sc}^*(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u \cdot d_v) d(u, v). \tag{5}$$

Finally, Gutman, in [24], introduced two topological polynomials, namely, the Schulz polynomial $\operatorname{Sc}(G, x)$ and the modified Schulz polynomial $\operatorname{Sc}^*(G, x)$ as follows:

$$\begin{aligned} \operatorname{Sc}(G, x) &= \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u + d_v) x^{d(u,v)}, \\ \operatorname{Sc}^*(G, x) &= \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u \cdot d_v) x^{d(u,v)}. \end{aligned} \tag{6}$$

The connection between the above polynomials and the previous two indices is stated below:

$$\begin{aligned} \operatorname{Sc}(G) &= \left.\frac{\partial \operatorname{Sc}(G, x)}{\partial x}\right|_{x=1}, \\ \operatorname{Sc}^*(G) &= \left.\frac{\partial \operatorname{Sc}^*(G, x)}{\partial x}\right|_{x=1}. \end{aligned} \tag{7}$$

1.2. Zero-Divisor Graphs. Let R be a commutative ring with nonzero identity and let $Z(R)$ be its set of zero divisors. The zero-divisor graph of R is the graph $\Gamma(R)$ with vertex set $V(\Gamma(R)) = Z(R)^*$, where $Z(R)^* = Z(R) \setminus \{0\}$, and edge set $E(\Gamma(R)) = \{\{x, y\}\colon\ x \cdot y = 0\}$. As usual, an edge $\{x, y\}$ is simply denoted as xy. Zero-divisor graphs were introduced by Beck [2] in 1988 and then studied by Anderson and Naseer in [26]. These authors were interested in colorings and the original definition included all elements in R, even the zero. Later on, Anderson and Livingston [27] made emphasis on the relationship between ring-theoretical properties and graph-theoretical properties and reformulated the definition as it appears in the lines above. One of the basic results in this relationship is the following one.

Theorem 1 (see [27]). *Let R be a commutative ring. Then, $\Gamma(R)$ is connected with diameter less or equal to 3.*

The study conducted in [28, 29] may serve as a survey that is very interesting to find the relation between ring-theoretic properties and graph-theoretic properties of $\Gamma(G)$. Some applications and relation between algebraic theory and chemical graph theory can be seen in [1, 18, 30]. In this paper, we presented some results that interplay in the relation between a zero-divisor graph and chemical graph theory. The structure of the paper is as follows. In Section 2, we describe the family of zero-divisor graphs of the form $\Gamma(\mathbb{Z}_{p^2q^2})$, where p and q are different primes, and we also count pairs of vertices that are exactly at distance i, for $i = 1, 2, 3$. In Section 3, we obtain the Wiener index and the Hosoya, the Shultz, and the modified Shultz polynomials of $\Gamma(\mathbb{Z}_{p^2q^2})$. We also obtain the Shultz and the modified Shultz indices of $\Gamma(\mathbb{Z}_{p^2q^2})$.

2. The Zero-Divisor Graph on $\Gamma(\mathbb{Z}_{p^2q^2})$

Let us start by introducing some notation that will be used along the paper. We assume that p and q are different positive primes.

Lemma 1. *Let $0 \leq i, j \leq 2$. Let $A_{i,j} = (p^i q^j) \subset \mathbb{Z}_{p^2q^2}$, for $0 \leq i + j \leq 4$ and $A_{i,j} = \varnothing$, otherwise. Then,*

(i) $|A_{i,j}| = p^{2-i} q^{2-j}$

(ii) $A_{i+1,j} \cup A_{i,j+1} \subset A_{i,j}$

(iii) $A_{i+1,j} \cap A_{i,j+1} = A_{i+1,j+1}$, whenever $i + j + 2 \leq 4$

The vertices of $\Gamma(\mathbb{Z}_{p^2q^2})$ can be split into blocks such that all vertices in the same block have the same behavior. From this partition, we can easily describe the structure of $\Gamma(\mathbb{Z}_{p^2q^2})$, that is, the content of the following lemma.

Lemma 2. *For $0 \leq i, j \leq 2$ and $0 < i + j < 4$, let $B_{i,j} = A_{i,j} \setminus (A_{i+1,j} \cup A_{i,j+1})$. Then,*

$$\left|B_{i,j}\right| = \begin{cases} p^{2-i}q^{2-j} - p^{1-i}q^{2-j} - p^{2-i}q^{1-j} + p^{1-i}q^{1-j}, & \text{if } \max\{i,j\} = 1, \\ q^{2-j} - q^{1-j}, & \text{if } i = 2, \\ p^{2-i} - p^{1-i}, & \text{if } j = 2. \end{cases} \tag{8}$$

Moreover,

(i) If $i, j \geq 1$, then $\Gamma[B_{i,j}]$ is a clique. Otherwise, $\Gamma[B_{i,j}]$ is a set of independent vertices.

(ii) Let $B_{i,j}$ and $B_{i',j'}$ such that $i + i' = j + j' = 2$. Then, the edges uv, $u \in B_{i,j}$ and $v \in B_{i',j'}$, define a complete bipartite graph.

According to the definition, all vertices in the same block of the zero-divisor graph on $\mathbb{Z}_{p^2q^2}$ have the same degree. For more details on this graph, see [30]. Let d_{ij} be the degree of any vertex in $B_{i,j}$. Following the notation of the previous lemma, we also conclude the following information.

Lemma 3. *For $0 \leq i, j \leq 2$ and $0 < i + j < 4$, then*

$$d_{ij} = \begin{cases} p^i q^j - i - j, & \text{if } \max\{i,j\} = 1, \\ p^2 q^j - j - 1, & \text{if } i = 2, \\ p^i q^2 - i - 1, & \text{if } j = 2. \end{cases} \tag{9}$$

Figure 1 shows the structure of the zero-divisor graph $\mathbb{Z}_{p^2q^2}$. White vertices represent blocks of independent vertices in $\mathbb{Z}_{p^2q^2}$, whereas black vertices represent cliques.

The structure shown in Lemmas 2 and 3 can be completed by showing the distance between pairs of vertices, which only depends on the block they belong to. This information appears in Table 1.

Let $\mathrm{TP}_i(G)$, $i \in \mathbb{Z}$ and $i > 0$, the number of pairs of vertices at distance i in a graph G.

Lemma 4. *Let $\Gamma(\mathbb{Z}_{p^2q^2})$ be a zero-divisor graph; then,*

$$\mathrm{TP}_1\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = 3pq(p-1)(q-1) + \frac{1}{2}(pq-1)(pq-2). \tag{10}$$

Proof. The size of $\Gamma(\mathbb{Z}_{p^2q^2})$ is given by

$$\left|B_{1,2}\right|\left(\left|B_{2,0}\right| + \left|B_{1,0}\right|\right) + \left|B_{2,1}\right|\left(\left|B_{0,2}\right| + \left|B_{0,1}\right|\right) + \left|B_{2,0}\right|\left|B_{0,2}\right| + \left|E\left(K_{|B_{1,2}|+|B_{1,1}|+|B_{2,1}|}\right)\right|. \tag{11}$$

That is, by introducing the values described in Lemma 2, the result follows. □

Lemma 5. *Let $\Gamma(\mathbb{Z}_{p^2q^2})$ be a zero-divisor graph; then,*

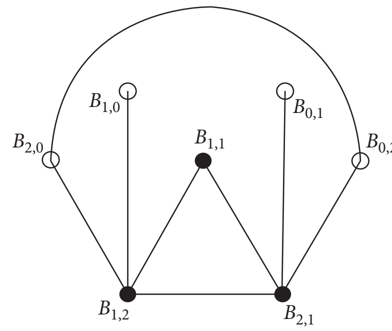

Figure 1: The structure of $\mathbb{Z}_{p^2q^2}$.

Table 1: Distance between pair of vertices, according to the block they belong to 1.

	$B_{1,0}$	$B_{0,1}$	$B_{2,0}$	$B_{1,1}$	$B_{0,2}$	$B_{1,2}$	$B_{2,1}$
$B_{1,0}$	2	3	2	2	3	1	2
$B_{0,1}$	3	2	3	2	2	2	1
$B_{2,0}$	2	3	2	2	1	1	2
$B_{1,1}$	2	2	2	1	2	1	1
$B_{0,2}$	3	2	1	2	2	2	1
$B_{1,2}$	1	2	1	1	2	1	1
$B_{2,1}$	2	1	2	1	1	1	1

$$\mathrm{TP}_2\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = \frac{1}{2}pq\left(pq\left(p^2 + q^2 - 6\right) + p + q + 2\right). \tag{12}$$

Proof. The number of pairs of vertices at distance 2 is given by the formula that follows:

$$\begin{aligned} \mathrm{TP}_2\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = {} & \binom{\left|B_{2,0}\right| + \left|B_{1,0}\right|}{2} + \binom{\left|B_{0,2}\right| + \left|B_{0,1}\right|}{2} \\ & + \left|B_{1,1}\right|\left(\left|B_{2,0}\right| + \left|B_{1,0}\right| + \left|B_{0,2}\right| + \left|B_{0,1}\right|\right) \\ & + \left|B_{2,1}\right|\left(\left|B_{2,0}\right| + \left|B_{1,0}\right|\right) + \left|B_{1,2}\right|\left(\left|B_{0,2}\right| + \left|B_{0,1}\right|\right), \end{aligned} \tag{13}$$

that is,

$$\begin{aligned} \mathrm{TP}_2\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = {} & \left(\left|B_{2,0}\right| + \left|B_{1,0}\right|\right)\left(\frac{\left|B_{2,0}\right| + \left|B_{1,0}\right| - 1}{2} + \left|B_{1,1}\right| + \left|B_{2,1}\right|\right) \\ & + \left(\left|B_{0,2}\right| + \left|B_{0,1}\right|\right)\left(\frac{\left|B_{0,2}\right| + \left|B_{0,1}\right| - 1}{2} + \left|B_{1,1}\right| + \left|B_{1,2}\right|\right). \end{aligned} \tag{14}$$

Thus, by Lemma 2, we obtain the following expression:

$$\mathrm{TP}_2\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = pq\left(\frac{p(q+2)(q-1) - 1}{2}(q-1) + \frac{q(p+2)(p-1) - 1}{2}(p-1)\right). \tag{15}$$

Hence, after simplification, the result follows. □

Lemma 6. *Let $\Gamma(\mathbb{Z}_{p^2q^2})$ be a zero-divisor graph; then,*

$$\mathrm{TP}_3\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = pq(p-1)(q-1)(pq-1). \tag{16}$$

Proof. The number of pairs at distance exactly 3, TP_3, is given by the following expression:

$$\mathrm{TP}_3\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = |B_{0,1}||B_{2,0}| + |B_{0,1}||B_{1,0}| + |B_{0,2}||B_{1,0}|. \tag{17}$$

Thus, by Lemma 2, we get the result. □

3. Distance-Based Topological Indices and Polynomials of $\Gamma(\mathbb{Z}_{p^2q^2})$

Now, we are ready to state and prove the following theorems.

Theorem 2. *The Winner index of $\Gamma(\mathbb{Z}_{p^2q^2})$ is*

$$W\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = 3p^2q^2(p-1)(q-1) + pq\left(pq\left(p^2+q^2-6\right)+p+q+2\right) + \frac{1}{2}(pq-1)(pq-2). \tag{18}$$

Proof. The diameter of $\Gamma(\mathbb{Z}_{p^2q^2})$ is 3. Thus, there are pairs of vertices at distance 1, 2, and 3, and the Winner index can be obtained as follows:

$$W\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = \mathrm{TP}_1 + 2\mathrm{TP}_2 + 3\mathrm{TP}_3. \tag{19}$$

By Lemmas 4–6, we get TP_1, TP_2, and TP_3, respectively. Thus, by introducing these values in (19), we get, after simplification, the required result. □

Lemma 7. *The Hosoya polynomial of $\Gamma(\mathbb{Z}_{p^2q^2})$ is $((p^2q^2-1)/2) + (TP_1)x + (TP_2)x^2 + (TP_3)x^3$.*

Theorem 3. *The Hosoya polynomial of $\Gamma(\mathbb{Z}_{p^2q^2})$ is*

$$\begin{aligned} H\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right), x\right) &= \frac{p^2q^2-1}{2} + \left(3pq(p-1)(q-1) + \frac{1}{2}(pq-1)(pq-2)\right)x \\ &\quad + \frac{1}{2}pq\left(pq\left(p^2+q^2-6\right)+p+q+2\right)x^2 \\ &\quad + pq(p-1)(q-1)(pq-1)x^3. \end{aligned} \tag{20}$$

Proof. The result follows by Lemma 7 and by Lemmas 4–6. □

Lemma 8. *The Hyper–Wiener index of $\Gamma(\mathbb{Z}_{p^2q^2})$ is $2TP_1 + 6TP_2 + 12TP_3$.*

Theorem 4. *The Hyper–Wiener index of $\Gamma(\mathbb{Z}_{p^2q^2})$ is*

$$WW\left(\Gamma\left(\mathbb{Z}_{p^2q^2}\right)\right) = 12p^2q^2(p-1)(q-1) + pq\left(pq\left(3p^2+3q^2-23\right)+9p+9q-3\right) + 2. \tag{21}$$

Proof. The result follows by Lemma 8 and by Lemmas 4–6, after some simplifications. □

Lemma 9. *Let $\alpha_{ij} = |B_{i,j}|d_{ij}$, where d_{ij} is the degree of any vertex in $B_{i,j}$, $0 \le i, j \le 2$ and $0 < i + j < 4$. Then, the Schultz polynomial of $\Gamma = \Gamma(\mathbb{Z}_{p^2q^2}) = (V, E)$ is equal to*

$$\begin{aligned} \mathrm{Sc}(\Gamma, x) &= \left\{\alpha_{10}\left(|B_{0,1}| + |B_{0,2}|\right) + \alpha_{01}\left(|B_{1,0}| + |B_{2,0}|\right) + \alpha_{20}|B_{0,1}| + \alpha_{02}|B_{1,0}|\right\}x^3 \\ &\quad + \left\{\left(|B_{0,1}| + |B_{0,2}|\right)(\alpha_{12}+\alpha_{11}) + \left(|B_{1,0}| + |B_{2,0}|\right)(\alpha_{21}+\alpha_{11}) + \left(d_{12} - |B_{1,2}|\right)(\alpha_{20}+\alpha_{10}) + \left(d_{21} - |B_{2,1}|\right)(\alpha_{02}+\alpha_{01})\right\}x^2 \\ &\quad + \sum_{u \in V(\Gamma)} d_u^2 x + 2|E(\Gamma)|. \end{aligned} \tag{22}$$

Proof. Since the diameter of Γ is 3, 3 is by definition the degree of $\mathrm{Sc}(\Gamma, x)$. The 3rd coefficient of the polynomial is given by

$$\left|B_{0,1}\right|\left|B_{1,0}\right|\left(d_{10}+d_{01}\right)+\left|B_{2,0}\right|\left|B_{0,1}\right|\left(d_{20}+d_{01}\right) + \left|B_{0,2}\right|\left|B_{1,0}\right|\left(d_{02}+d_{10}\right). \quad (23)$$

That is, $\alpha_{10}|B_{0,1}| + \alpha_{01}|B_{1,0}| + \alpha_{20}|B_{0,1}| + \alpha_{01}|B_{2,0}| + \alpha_{02}|B_{1,0}| + \alpha_{10}|B_{0,2}|$. From this expression, we clearly obtain the 3rd coefficient that appears in the statement.

The coefficients of x^2 and x (see Table 1) are given, respectively, by

$$\begin{aligned} s_2 = {} & 2\binom{|B_{1,0}|}{2}d_{10} + 2\binom{|B_{2,0}|}{2}d_{20} + 2\binom{|B_{0,1}|}{2}d_{01} + 2\binom{|B_{0,2}|}{2}d_{02} \\ & +|B_{2,0}||B_{1,0}|(d_{20}+d_{10}) + |B_{1,1}||B_{1,0}|(d_{11}+d_{10}) + |B_{1,1}||B_{0,1}|(d_{11}+d_{01}) \\ & +|B_{1,1}||B_{2,0}|(d_{11}+d_{20}) + |B_{0,2}||B_{0,1}|(d_{02}+d_{01}) + |B_{0,2}||B_{1,1}|(d_{02}+d_{11}) \\ & +|B_{1,2}||B_{0,1}|(d_{12}+d_{01}) + |B_{1,2}||B_{0,2}|(d_{12}+d_{02}) + |B_{2,1}||B_{1,0}|(d_{21}+d_{10}) \\ & +|B_{2,1}||B_{2,0}|(d_{21}+d_{20}), \\ s_1 = {} & 2\binom{|B_{1,1}|}{2}d_{11} + 2\binom{|B_{1,2}|}{2}d_{12} + 2\binom{|B_{2,1}|}{2}d_{21} + |B_{1,2}||B_{2,0}|(d_{12}+d_{20}) \\ & +|B_{2,1}||B_{0,2}|(d_{21}+d_{02}) + |B_{1,2}||B_{1,0}|(d_{12}+d_{10}) + |B_{2,1}||B_{0,1}|(d_{21}+d_{01}) \\ & +|B_{0,2}||B_{2,0}|(d_{02}+d_{20}) + |B_{1,1}||B_{1,2}|(d_{11}+d_{12}) + |B_{1,1}||B_{2,1}|(d_{11}+d_{21}) \\ & +|B_{2,1}||B_{1,2}|(d_{21}+d_{12}). \end{aligned} \quad (24)$$

By doing similar transformations as above, we obtain the 2^n and the 1st coefficient, respectively, that appears in the statement. Finally, the independent term appears when we apply the formula to each vertex. □

Theorem 5. *Let p and q be different primes. Then, the Schultz polynomial of $\Gamma = \Gamma(\mathbb{Z}_{p^2q^2})$ is equal to*

$$\begin{aligned} \mathrm{Sc}(\Gamma, x) = {} & \left\{p(p-1)q(q-1)\left(2p^2q + 2pq^2 - 4pq - p^2 - q^2 + 2\right)\right\}x^3 \\ & + \left\{pq\left(4p^3q^2 + 4p^2q^3 - 3p^3q - 12p^2q^2 - 3pq^3 + 2pq^2 + 2p^2q + 6pq + 2p^2 + 2q^2 - 4\right)\right\}x^2 \\ & + \Big\{(p-1)(q-1)\left(p^3q + p^2q^2 + pq^3 + 2p^2q + 2pq^2 - 10pq + 4\right) + (p-1)\left(pq^2 - 2\right)^2 \\ & + (q-1)\left(pq^2 - 2\right)^2\Big\}x + (p-1)(q-1)(5pq-2) + (p-1)\left(pq^2 - 2\right) \\ & + (q-1)\left(p^2q - 2\right). \end{aligned} \quad (25)$$

Proof. Consider the formula obtained in Lemma 9. Note that

$$\sum_{u \in V(\Gamma)} d_u^2 = \alpha_{20}d_{20} + \alpha_{02}d_{02} + \alpha_{10}d_{10} + \alpha_{01}d_{01} + \alpha_{11}d_{11} + \alpha_{12}d_{12} + \alpha_{21}d_{21} \quad (26)$$

and $2|E(\Gamma)| = \alpha_{20} + \alpha_{02} + \alpha_{10} + \alpha_{01} + \alpha_{11} + \alpha_{12} + \alpha_{21}$. By introducing the values of $|B_{i,j}|$, d_{ij} (collected in Lemmas 2 and 3), and α_{ij} in terms of p and q, the result follows. □

Corollary 1. *The Schultz index or the degree distance of $\Gamma = \Gamma(\mathbb{Z}_{p^2q^2})$ is equal to*

$$\begin{aligned}\mathrm{Sc}(\Gamma,x) = {} & 3p(p-1)q(q-1)\left(2p^2q+2pq^2-4pq-p^2-q^2+2\right)+2pq \\ & \cdot\left(4p^3q^2+4p^2q^3-3p^3q-12p^2q^2-3pq^3+2pq^2+2p^2q+6pq+2p^2+2q^2-4\right) \\ & +(p-1)(q-1)\left(p^3q+p^2q^2+pq^3+2p^2q+2pq^2-10pq+4\right)+(p-1)\left(pq^2-2\right)^2 \\ & +(q-1)\left(pq^2-2\right)^2.\end{aligned} \tag{27}$$

Lemma 10. *Let $\alpha_{ij}=|B_{i,j}|d_{ij}$, where d_{ij} is the degree of any vertex in $B_{i,j}$, $0\le i,j\le 2$ and $0<i+j<4$. Then, the modified Schultz polynomial of $\Gamma=\Gamma(\mathbb{Z}_{p^2q^2})=(V,E)$ is equal to*

$$\begin{aligned}\mathrm{Sc}^*(\Gamma,x) = {} & \{\alpha_{10}\alpha_{01}+\alpha_{20}\alpha_{01}+\alpha_{02}\alpha_{10}\}x^3+\left\{\frac{\alpha_{10}(\alpha_{10}-d_{10})}{2}+\frac{\alpha_{20}(\alpha_{20}-d_{20})}{2}\right. \\ & +\frac{\alpha_{01}(\alpha_{01}-d_{01})}{2}+\frac{\alpha_{02}(\alpha_{02}-d_{02})}{2}+\alpha_{20}\alpha_{10}+\alpha_{11}\alpha_{10}+\alpha_{11}\alpha_{01}+\alpha_{11}\alpha_{20}+ \\ & \left.+\alpha_{02}\alpha_{01}+\alpha_{02}\alpha_{11}+\alpha_{12}\alpha_{01}+\alpha_{12}\alpha_{02}+\alpha_{21}\alpha_{10}+\alpha_{21}\alpha_{20}\right\}x^2+\left\{\frac{\alpha_{11}(\alpha_{11}-d_{11})}{2}\right. \\ & +\frac{\alpha_{12}(\alpha_{12}-d_{12})}{2}+\frac{\alpha_{21}(\alpha_{21}-d_{21})}{2}+\alpha_{12}\alpha_{20}+\alpha_{21}\alpha_{02}+\alpha_{12}\alpha_{10}+\alpha_{21}\alpha_{01} \\ & \left.+\alpha_{02}\alpha_{20}+\alpha_{11}\alpha_{12}+\alpha_{11}\alpha_{21}+\alpha_{21}\alpha_{12}\right\}x+\sum_{u\in V}d_u^2.\end{aligned} \tag{28}$$

Proof. Since the diameter of Γ is 3, 3 is by definition the degree of $\mathrm{Sc}^*(\Gamma,x)$. The 3rd coefficient of the polynomial is given by

$$|B_{0,1}||B_{1,0}|d_{10}d_{01}+|B_{2,0}||B_{0,1}|d_{20}d_{01}+|B_{0,2}||B_{1,0}|d_{02}d_{10}, \tag{29}$$

that is, $\alpha_{10}\alpha_{01}+\alpha_{20}\alpha_{01}+\alpha_{02}\alpha_{10}$.

The coefficients of x^2 and x (see Table 1) are given, respectively, by

$$\begin{aligned} s_2^* = {} & \binom{|B_{1,0}|}{2}d_{10}^2+\binom{|B_{2,0}|}{2}d_{20}^2+\binom{|B_{0,1}|}{2}d_{01}^2+\binom{|B_{0,2}|}{2}d_{02}^2+|B_{2,0}||B_{1,0}|d_{20}d_{10} \\ & +|B_{1,1}||B_{1,0}|d_{11}d_{10}+|B_{1,1}||B_{0,1}|d_{11}d_{01}+|B_{1,1}||B_{2,0}|d_{11}d_{20}+|B_{0,2}||B_{0,1}|d_{02}d_{01} \\ & +|B_{0,2}||B_{1,1}|d_{02}d_{11}+|B_{1,2}||B_{0,1}|d_{12}d_{01}+|B_{1,2}||B_{0,2}|d_{12}d_{02}+|B_{2,1}||B_{1,0}|d_{21}d_{10} \\ & +|B_{2,1}||B_{2,0}|d_{21}d_{20}, \\ s_1^* = {} & \binom{|B_{1,1}|}{2}d_{11}^2+\binom{|B_{1,2}|}{2}d_{12}^2+\binom{|B_{2,1}|}{2}d_{21}^2+|B_{1,2}||B_{2,0}|d_{12}d_{20} \\ & +|B_{2,1}||B_{0,2}|d_{21}d_{02}+|B_{1,2}||B_{1,0}|d_{12}d_{10}+|B_{2,1}||B_{01}|d_{21}d_{01}+|B_{0,2}||B_{2,0}|d_{02}d_{20} \\ & +|B_{1,1}||B_{1,2}|d_{11}d_{12}+|B_{1,1}||B_{2,1}|d_{11}d_{21}+|B_{2,1}||B_{1,2}|d_{21}d_{12}.\end{aligned} \tag{30}$$

By doing similar transformations as above, we obtain the 2^n and the 1st coefficient, respectively, that appears in the statement. Finally, the independent term appears when we apply the formula to each vertex. □

Theorem 6. *Let p and q be different primes. Then, the modified Schultz polynomial of $\Gamma = \Gamma(\mathbb{Z}_{p^2q^2})$ is equal to*

$$\begin{aligned}
\mathrm{Sc}^*(\Gamma, x) &= \left\{p(p-1)^2 q(q-1)^2(3pq-p-q-1)\right\}x^3 \\
&+ \Bigg\{(p-1)^2(q-1)^2\left(8p^2q^2 + \frac{(p^2q+pq^2)}{2} - p^2 - q^2 - 11pq - p - q\right) \\
&+ \frac{1}{2}(p-1)(q-1)\big(6p^3q^3 - 2p^3q - 2pq^3 - 6p^2q^2 - 4p^2q - 4pq^2 - p^3 - q^3 - 3p^2 \\
&- 3q^2 + 10pq + 5p + 5q\big)\Bigg\}x^2 + \Big\{(p-1)(q-1)\big(13p^3q^3 - 5p^3q^2 - 2p^3q - p^2q^3 \\
&- 8p^2q^2 - 8p^2q - 6pq^3 - 4pq^2 + 14pq + 4p + 4q\big) + \frac{1}{2}(p-1)(p-2)\left(pq^2-2\right)^2 \\
&+ \frac{1}{2}(q-1)(q-2)\left(p^2q-2\right)^2\Big\}x + (p-1)\left(pq^2-2\right)^2 + (q-1)\left(pq^2-2\right)^2 \\
&+ (p-1)(q-1)\left(p^3q + p^2q^2 + pq^3 + p^2q + pq^2 - 8pq + 4\right).
\end{aligned} \tag{31}$$

Proof. Consider the formula obtained in Lemma 10. Recall that $\sum_{u\in V(\Gamma)} d_u^2 = \alpha_{20}d_{20} + \alpha_{02}d_{02} + \alpha_{10}d_{10} + \alpha_{01}d_{01} + \alpha_{11}d_{11} + \alpha_{12}d_{12} + \alpha_{21}d_{21}$. By introducing the values of $|B_{i,j}|$, d_{ij} (collected in Lemmas 2 and 3), and α_{ij} in terms of p and q, the result follows. □

Corollary 2. *The modified Schultz index of $\Gamma = \Gamma(\mathbb{Z}_{p^2q^2})$ is equal to*

$$\begin{aligned}
\mathrm{Sc}(\Gamma, x) &= (p-1)^2(q-1)^2\left(25p^2q^2 - 2p^2q - 2pq^2 - p^2 - q^2 - 14pq - p - q\right) \\
&+ (p-1)(q-1)\big(19p^3q^3 - 5p^3q^2 - 4p^3q - p^3 - 14p^2q^2 - 12p^2q - 3p^2 - 8pq^3 \\
&- 8pq^2 + 24pq + 9p - q^3 - 3q^2 + 9q\big) + \frac{1}{2}(p-1)(p-2)\left(pq^2-2\right)^2 \\
&+ \frac{1}{2}(q-1)(q-2)\left(p^2q-2\right)^2.
\end{aligned} \tag{32}$$

4. Conclusion

The structure of zero-divisor graphs of the form of $\Gamma(\mathbb{Z}_{p^2q^2})$ is particularly interesting for studying distance-based topological indices. First, because its diameter is exactly 3, but also because there are defined blocks, with a complete bipartite connection between them, of either independent vertices or complete graphs (cliques). In this paper, we have focused on the Wiener index and the Hosoya, the Shultz, and the modified Shultz polynomials of $\Gamma(\mathbb{Z}_{p^2q^2})$ and, finally, on the Shultz and the modified Shultz indices of $\Gamma(\mathbb{Z}_{p^2q^2})$. For that reason, we have introduced some notation that could be useful not only for studying other distance-base topological indices of $\Gamma(\mathbb{Z}_{p^2q^2})$ but also for other graphs of the form $\Gamma(\mathbb{Z}_{p^mq^n})$, for m, n positive integers. A key point in this notation is the study of pairs that are exactly a distance one (the size of the graph), two, or three. We think that a possible line of future research should include the study of paths connecting pairs of vertices a different distances and the extension to other indices, as for instance, the Estrada index.

Data Availability

All the data are provided within the manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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